

Final Program
 NLCat 2000
 Advanced Photon Source
 Argonne National Laboratory
 October 12-13, 2000

<i>Thursday, October 12</i>		
7:00 a.m.	Registration	
8:30 a.m.	Welcome	
8:45 a.m.	APS Auditorium - Keynote #1 - Professor Gabor A. Somorjai, Lawrence Berkeley National Laboratory, "Surface Science in Catalysis, from Vacuum to In Situ Studies"	
9:30 a.m.	Coffee Break	
Breakout Sessions		
	Room - E1100/1200	APS Auditorium
Moderators	Daniel DuBois (NREL)	Kathleen Carrado (ANL)
9:45 a.m.	A1 - "Development of an Embedded Cluster Model for Studies of Chemical Processes in Imperfect Crystals" – <u>M. Gutowski</u> , J. E. Jaffe, PNNL; S. Derenzo, LBNL	B1 - "The Synchrotron Consortium for Catalytic Research" – D. R. Mullins, ORNL; J. G. Chen, M. A. Bartreau, R. F. Lobo, The University of Delaware; C.-C. Kao, S. Hulbert, J. Hrbek, D. P. Siddons, J. A. Rodriguez, BNL
10:15 a.m.	A2 - "Dense Monolayer Adsorption of Monovalent Metals on CaO and MgO (100) Surfaces: A Theoretical Study" – D. R. Alfonso, <u>J. E. Jaffe</u> , A. C. Hess and M. Gutowski, PNNL	B2 - "In-situ Ultraviolet Raman Spectroscopy of Advanced Catalysts" – <u>J. W. Ager III</u> , C. Tewell and G. Somorjai, LBNL; F. Malizia, Montell Italia, Italy
10:45 a.m.	A3 - "Computational Studies of Olefin Epoxidation" – <u>M. R. Salazar</u> , J. D. Kress, and A. Redondo, LANL	B3 - "The Role of Cobalt in (Co)MoS₂ Hydrodesulfurization Catalysts" – <u>A. J. Kropf</u> , C. L. Marshall, ANL; J. T. Miller, BP Chemicals
11:15 a.m.	A4 - "Towards a Device-Scale Model for Catalytic Converters" – <u>K. Chakravarthy</u> , J. Conklin, S. Daw, E. D'Azevedo, ORNL	B4 - "Nanophase Support Materials as Catalysts for Ultra-Deep Sulfur Removal from Crude Oil and Transportation Fuels" – <u>D. Mahajan</u> , BNL; C. L. Marshall, ANL
11:45 a.m.	A5 - "Challenges in Lean-Burn Automotive Exhaust Catalysis" – T. J. Gardner, L. I. McLaughlin, <u>D. L. Mowery</u> and R. S. Sandoval, SNL	B5 - "Hydrodesulfurization Activity and Selectivity of MCM-41 Support Catalysts" – <u>C. L. Marshall</u> , D. Wei, L. Ruscic, L. Xu and K. Carrado, ANL
12:15 p.m.	Group Luncheon	

1:00 p.m.	APS Gallery - Luncheon Address #1 - Professor Peter Stair, Director, Center for Catalysis, Northwestern University, "Northwestern University Institute for Environmental Catalysis "	
1:45 p.m.	APS Auditorium - Keynote #2 - Dr. Suresh Sriramulu, A D Little, "Microkinetics Modeling in Catalysis"	
	Room – E1100/1200	APS Auditorium
Moderators	Morris Bullock (BNL)	Daniel Ginosar (INEEL)
2:15 p.m.	A6 - “Reduction of NO_x Emissions in Lean-Burn Engine Exhaust with Novel Zeolite-Based Materials” – <u>N. C. Clark</u> and K. C. Ott, LANL	B6 - “Structural Changes in Metal Molybdates During Dehydration, Desulfurization, and Oxidation Determined from In-situ Time-resolved Synchrotron X-ray Powder Diffraction” – <u>J. C. Hanson</u> and J. Rodriguez, BNL
2:45 p.m.	A7 – “Metal-Superoxo and Metal-Oxo Complexes as Intermediates in Catalytic Oxidations by Molecular Oxygen” – <u>A. Bakac</u> , Ames Lab.	B7 - “Structurally Ordered Magnesium Vanadate Model Catalysts for Oxidative Dehydrogenation” – A. G. Sault, J. E. Mudd, J. A. Ruffner and <u>J. E. Miller</u> , SNL
3:15 p.m.	A8 - “Synthetic Oxotransferases: Oxorhenium Compounds in Catalysis” – <u>J. H. Espenson</u> , Ames Lab.	B8 - “Defect Characterization on MgO(100) Using Adsorption of Small Molecules” – Z. Dohnalek, G. A. Kimmel, P. Ayotte, R. S. Smith, S. A. Joyce, and B. D. Kay, PNNL
3:45 p.m.	Break	
4:00 p.m.	A9 - “Oxidative Dehydrogenation of Ethane over Phosphate Catalysts” – <u>J. E. Miller</u> , M. M. Gonzales, L. Evans, L. D. Mansker, SNL; C. Zhang, R. Rao, G. Whitwell, Akzo Nobel; A. Maiti, D. King-Smith, P. Kung, J. Newsam, Molecular Simulations	B 9 -“Interfaced Controlled, Self-Assembled Cu₂O Quantum Dots as Novel Photocatalysts” – <u>Y. Liang</u> , Y. Su, J. Daschbach, D. McCready, S. Thevuthasan, V. Shutthanandan, PNNL; P. Meethunkij, Yale Univ.
4:30 p.m.	A10 - “Catalytic Oxo-Transfer Reactions Involving Imidomethylrhenium-Oxo and Peroxo Complexes” – <u>W.-D. Wang</u> and J. E. Espenson, Ames Lab	B10 -“Interaction of Water With Epitaxial Anatase-TiO₂(001) Thin Films” – <u>G. S. Herman</u> , M. A. Henderson, and Y. Gao, PNNL
5:30 p.m.	Poster Session and Reception - APS Gallery	
7:00 p.m.	Dinner - Argonne Guest House	

Poster Session and Reception - Thursday, October 12, 2000, 5:30 - 7:00 p.m.

P1	"Oxidative Dehydrogenation of Ethane Over VO/ZSM-5 and Phosphate Catalysts" – C. Zhang, A. Kraft, R. Rao, G. Whitwell, Akzo Nobel; J. E. Miller, M. M. Gonzales, L. Evans, L. D. Mansker, SNL; A. Maiti, D. King-Smith, P. Kung, J. Hewsam, Molecular Simulations, Inc.
P2	"Reactions Between Co-adsorbates on Model Emission Control Catalysts" – D. R. Mullins and S. H. Overbury, ORNL
P3	"Fundamental Studies of the Formation of Synthetic Clay Catalysts" – K. A. Carrado, L. Xu, S. Seifert, R. E. Botto, ANL; D. Gregory, Quantum Magnetics; K. Song, Novellus Systems
P4	"Bifunctional Catalysts for Selective NO_x Reduction" – M. K. Neylon, C. L. Marshall, ANL; L. C. Satek, M. E. Carrera, BP Chemicals
P5	"Investigations of the Reaction of Ethane/Oxygen/Hydrogen Mixtures on Platinum Catalysts in a Stagnation Flow Reactor" – A. H. S. F. Rice, M. D. Allendorf, SNL; D. K. Zerkle, LANL
P6	"Chemistry of Thiophene, H₂S, and SO₂ on Carbide-Modified Mo(110) and Mo₂C Powders" – J. A. Rodriguez, J. Dvorak and T. Jirsak, BNL
P7	"New Catalyst Technology for the Direct Oxidation of Benzene to Phenol" – C. Hamilton, E. A. Gardner, L. E. Iton, C. L. Marshall, ANL; S. Alerasool, P. E. Mayurinik, Engelhard Corporation; P. C. Y. Yeh, F. M. Dautzenberg, R. Overbeek, ABB Lummus; G. McRae, E. Meeks, Reaction Design; M. Neurock, University of Virginia; H. H. Kung and K. Popp, Northwestern University
P8	"Chemistry of Tris(allyl)Iridium: Towards a Composite Membrane for Low Temperature Alkane Dehydrogenation" – K. D. John, D. R. Pesiri, R. C. Dye, A. P. Sattelberger, and R. T. Baker, LANL
P9	"Characterization of Small Metal Particles on Planar Model Oxide Supports Using Scanning Tunneling Microscopy" – G. W. Zajac, BP Amoco; C. Xu, X. Lai and D. W. Goodman, Texas A&M University
P10	"Selective Oxidation of C₄ Hydrocarbons Over Mixed Metal Oxides" – G. L. Schrader, Ames Laboratory
P11	"Nano-Sized Pt Clusters on TiO₂ Rutile Surfaces: Growth, Self-Organization, and Chemisorption" – Y. Liang, S. Gan, D. Baer, M. Sievers, G. Herman, C. Peden, PNNL
P12	"Progress in Applications of High Resolution Solid State NMR to Catalysis" – M. Pruski, Ames Laboratory
P13	"Reaction Dynamics and Kinetics on Polycrystalline Ag" – R. J. Behuler and M. G. White, BNL
P14	"Rapid Catalysts Discovery for Selective Oxidation of Hydrocarbons for Form Oxygenates and Higher Hydrocarbons" – R. J. Evans and Kimberly A. Magrini-Bair, NREL
P15	"Catalytic Autothermal Reforming of Hydrocarbons for Fuel Cell Applications" – Y. Shi, C. Cioffi, S. Gao, and P. Chintawar, Nurvera Fuel Cells
P16	"Recent Advances in Petroleum Oils Conversion Biocatalysis" – M. S. Lin and E. T. Premuzic, BNL
P17	"The Advanced Technology Program" – R. A. Beyerlein, R. Bloksberg-Fireovid and J. D. Hewes, NIST
P18	"Photocatalyst for the Production of Methanol from Methane and Water Using Visible Light" – C. E. Taylor, NETL
P19	"Computational Studies of Potential Energy Surfaces for Hydrocarbon Reactions in Cluster Models of Zeolite H-ZSM-5" – S. A. Zygmunt, Valparaiso University; P. Zapol, L. A. Curtiss, L. E. Iton, ANL
P20	"Catalysis in the Office of Basic Energy Sciences, U.S. Department of Energy" – P. H. Smith, Office of Basic Energy Sciences, DOE, Washington, DC

Friday, October 13

8:30 a.m.	APS Auditorium - Keynote #3 - <u>Harold Kung</u> , Northwestern University, "Oxidative Reforming of Methanol and Hydrocarbon Cracking on Acidic Zeolite: Examples of Collaborative Research at Northwestern University "	
9:30 a.m.	Coffee Break	
Break out Sessions		
	Room – E1100/1200	APS Auditorium
Moderators	Robert Klingler (ANL)	Timothy Gardner (SNL)
9:45 a.m.	A11 - “Iridium-Catalyzed Selective Oxidation of Aryl Alkanones to Benzaldehyde” – <u>J. A. Franz</u> , D. S. Kolwaite, J. C. Linehan, and D. M. Camaioni, PNNL	B11 - “Development of New Catalysts for Reforming Hydrocarbon Feedstocks” – <u>T. R. Krause</u> , J. D. Carter, J. P. Kopasz, J.-M. Bae, S. Ahmed, and M. Krumpelt, ANL
10:15 a.m.	A12 - “Catonic Precious Metal Phosphonium Complexes for Bifunctional Catalysis” – M. B. Abrams, <u>R. T. Baker</u> , R. L. Martin, K. D. John, LANL	B12 - “Catalyst Development for Fuel Processing Applications in Microchannel Catalytic Reactors” – Y. Wang, <u>J. Hu</u> , D. P. VanderWiel, Y.-H. Chin, D. R. Palo, S. T. Perry, R. T. Rozmiarek, A. Y. Tonkovich, and E. G. Baker, PNNL
10:45 a.m.	A13 - “Catalytic Ionic Hydrogenations: Hydrogenation of Ketones and Dehydroxylation of Diols” – <u>R. M. Bullock</u> , M. H. Voges, M. Schlaf, B. F. M. Kimmich, P. Ghosh, E. Hauptman and P. J. Fagan, BNL & DuPont	B13 - “Reducibility of Model Catalytic Converter Oxygen Storage Materials: Thin Ce_xZr_{2-x}O₂(111) Films Grown on Y-Stabilized Zirconia Single Crystals” – <u>C. H. F. Peden</u> , T. He, G. S. Herman, Y. Gao, and S. Thevuthasan, PNNL; Y.-J. Kim, Taejon National University, S. Korea
11:15 a.m.	A14 - “Transient FTIR Study of the Re(dmb)(CO)₃· Radical Reactions in Photochemical CO₂ Reduction” – <u>E. Fujita</u> , K. Shinozaki, and B. S. Brunschwig, BNL	B14 - “DeSO_x and DeNO_x Reactions on Oxides” – <u>J. A. Rodriguez</u> , T. Jirsak, J. Dvorak, J. Hrbek, and J. Z. Larese, BNL
11:45 a.m.	A15 - “High-Pressure NMR Characterization of Micellar Systems for Catalysis” – <u>R. Klingler</u> , D. Fremgen, R. Gerald II, and J. Rathke, ANL	B15 - “Plasma Catalytic Lean NO_x Reduction with Zeolite and Alumina Catalysts” – <u>M. L. Balmer</u> , A. Panov, S. Yoon, A. Kolwaite and R. Tonkyn, PNNL
12:15 p.m.	Group Luncheon	

1:00 p.m.	APS Gallery - Luncheon Address #2 -Dr. Ronald Yates, Dow Chemical Company, "How to Have a Successful Industry-National Laboratory Interaction"	
	Room – E1100/1200	APS Auditorium
Moderators	Michael Chen (ANL)	Charles Peden (PNNL)
1:45 p.m.	A16 - “Phase-Separable Catalysis Approaches Using Supercritical Carbon Dioxide” – F. Liu, G. Jacobson, <u>B. Tumas</u> , LANL	B16 - “In-situ Filtration of Fischer-Tropsch Product Wax from Iron-based Catalysts” – <u>R. J. Gormley</u> , M. F. Zarochak, Natl. Energy Tech. Lab.; P. W. Deffenbaugh, Parsons Project Services, NETL
2:15 p.m.	A17 - “High-Pressure NMR Studies of Supercritical Carbonylation Catalysis” – <u>J. W. Rathke</u> , R. J. Klingler, M. J. Chen, L. M. Wojcinski, ANL	B17 - “Detailed Modeling of Ethane Partial Oxidation at Millisecond Contact Times” – <u>D. K. Zerkle</u> , LANL; M. D. Allendorf, SNL
2:45 p.m.	A18 - “Development of a Hydride Donor Scale and Its Application to Catalysis” – <u>D. L. DuBois</u> , D. E. Berning, A. Miedaner, C. J. Curtis, and W. W. Ellis, NREL	B18 - “Sustainable Solid-Acid Isoparaffin Alkylation Using Supercritical Fluids” – <u>D. M. Ginosar</u> , D. N. Thompson, K. Coates, INEEL
3:15 p.m.	A19 - “Free Radical Reactivity of Transition Metal Hydrides and Metal Cluster Thiols. Kinetics and Density Functional Theoretical Treatment of Radicals and Closed Shell Species” – <u>J. A. Franz</u> , D. S. Kolwaite, J. C. Linehan, J. C. Birnbaum, PNNL; E. Rosenberg, Univ. of Montana; J. Look and K. I. Goldberg, Univ. of Washington	B19 - “Mesoporous Silica Supported Solid Acid” – S. Choi, Y. Wang, K.-Y. Lee, and <u>C. H. F. Peden</u> , PNNL